Los Alamos National Laboratory
Applied Theoretical and Computational Physics Division
Research Note XCI-RN(U)98-041 (LA-UR-98-5718)
December 1998

ENDF/B-VI Neutron Library for MCNP with Probability Tables

Robert C. Little
X-CI; Code Integration Group

Robert E. MacFarlane
T-2; Applied Theoretical and Nuclear Physics

Executive Summary

A neutron cross-section library that includes probability tables to represent unresolved resonances is available for use in MCNP. The name of the library is URES. Room-temperature data for 27 isotopes are provided, based on ENDF/B-VI release 4. URES is compatible with versions of MCNP beginning with 4XS. This Research Note documents the creation, verification, and utilization of the URES library.

Introduction

Versions of MCNP™ up through and including Version 4B[1] have treated neutron cross sections in the unresolved energy range as if they were infinitely dilute. The energy-dependent cross sections in this energy range, therefore, have been relatively smooth, without any substantial fluctuations or resonance structure. The result has been that neutron self-shielding effects in the unresolved energy region have not been accurately modeled with MCNP.

Figure 1 illustrates the ENDF/B-V radiative capture cross section for ^{238}U as a function of neutron energy. The energy region between the vertical dashed lines (from 4 keV to 149 keV) is the unresolved resonance region as defined by this particular evaluation. As can be seen, there appears to be an abrupt transition at 4 keV from detailed resonance behavior to a smooth cross section.

In reality, the lack of structure exhibited in Figure 1 in the unresolved energy region is not physical. In fact, resonance behavior *does* extend to higher energies. However, resolved resonance structure is generally not extended to these higher energies in most nuclear data evaluations. The major reason for this omission is that the resolution of available experimental data is such that individual resonances can no longer be well defined at these energies. In addition, the practicality of including such explicit data eventually becomes prohibitive.

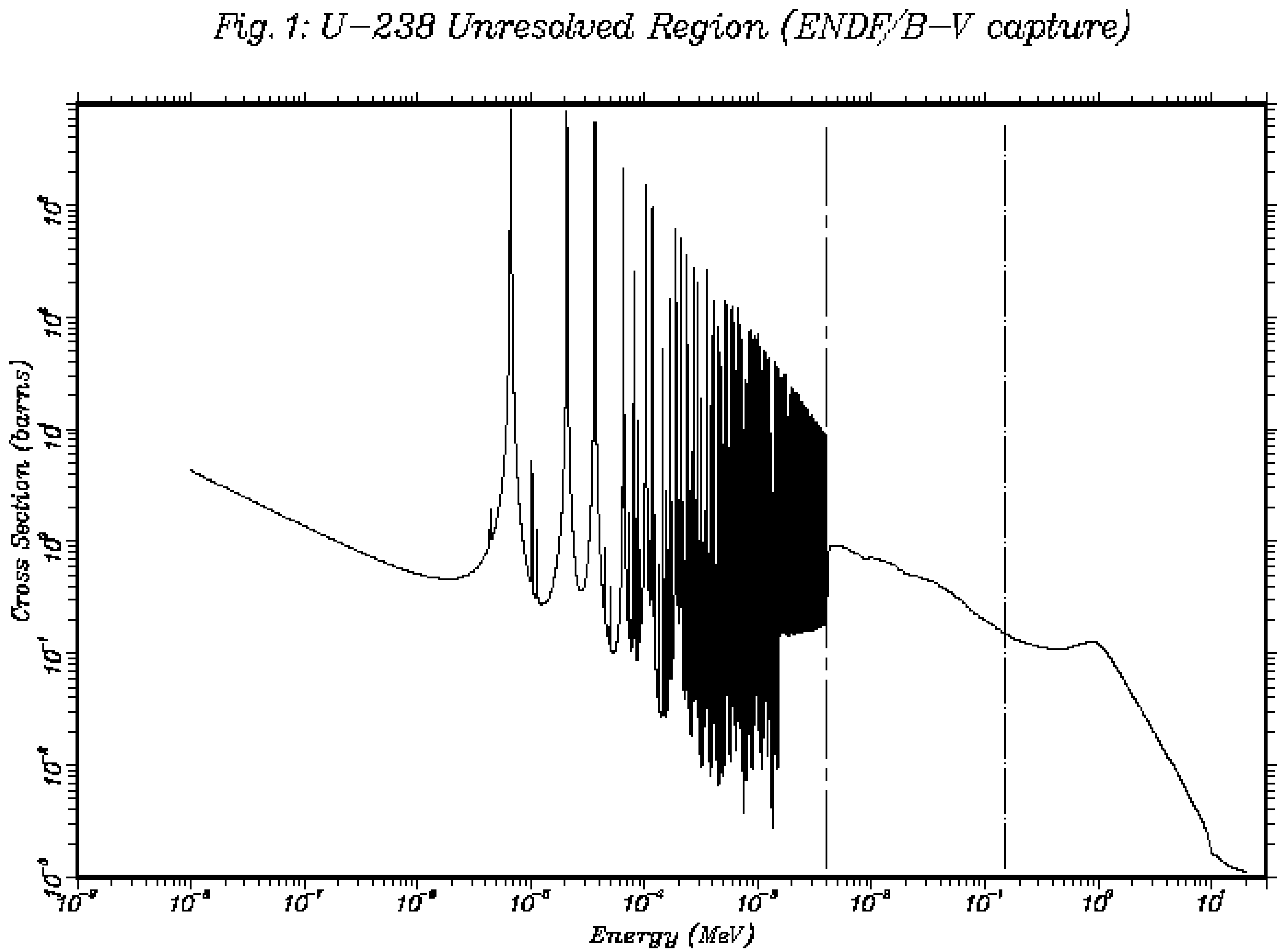
Often times, nuclear data evaluations *do* include information describing the distribution of resonance behavior in the unresolved region. For example, the ENDF format[2] allows evaluators to provide average level spacings and average neutron, radiative, fission, and competitive widths (all as a function of neutron energy) over the unresolved region. It has generally been the *average* (also referred to as the smooth, or unshielded, or infinitely dilute) cross sections determined from these parameters that MCNP has used.

One approach that has been implemented in continuous-energy Monte Carlo neutron transport codes to account statistically for the average resonance parameters specified in the unresolved resonance range is the probability table (PT) method.[3] In this method, the average parameters are used to generate ladders of representative resonances. Cross sections from these ladders are then used to form cross-section probability distribution functions, from which a table of cross sections (total, elastic, fission, and radiative capture) as a function of probability is prepared. When transporting neutrons in the unresolved energy range of a particular nuclide, the Monte Carlo code samples the total and reaction cross sections at the energy of the neutron, rather than simply using single average values at this energy. The PT method has been available in the VIM Monte Carlo code for some time.[4] More recently, it has also been implemented in the RACER[5] and TRIPOLI[6] codes.

MCNP has also been upgraded to incorporate the PT method. The implementation is described in Ref. 7. Specifics concerning the first version of MCNP to be released with the PT method (Version 4XS) are provided in Ref. 8.

In parallel with the efforts to upgrade MCNP, a new MCNP neutron cross-section library (named URES) has also been developed. The library provides data for 27 isotopes based on ENDF/B-VI Release 4.[9] This is the first time that PT data have been incorporated in an

™ MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory.



MCNP library. Data on the library have been processed by NJOY.[10] All cross sections on the library have been processed at room temperature (300 degrees Kelvin). The MCNP ZAIDs of all cross-section tables on URES end in .49c.

The remainder of this Research Note documents the creation, verification, and utilization of the URES library, including a concern about heating numbers in the probability tables. The following sections describe the ENDF/B evaluations used, the NJOY processing techniques, and the verification efforts. Then, the actual MCNP library is discussed, along with how to use it in MCNP. Relationships to data on other MCNP libraries will be described. Finally, selected calculational results will be presented.

Evaluation Sources

This work commenced by processing 29 ENDF/B-VI evaluations. The 29 materials selected for processing represent a subset of the ENDF/B-VI evaluations that include unresolved resonance data. The specific materials for this work were selected based upon their perceived importance in nuclear criticality safety applications. Note that MCNP data tables from two evaluations, Mo and ^{181}Ta, were ultimately discarded. See the section below on verification for details on why this was the case.

Table I gives information about the source of each evaluation used in this work. In particular, the ENDF/B-VI Release used as the evaluation source is specified for each of the 29 materials processed.

Table I

Materials and ENDF/B-VI Releases of Evaluations Used

Material	ENDF/B-VI Release	Material	ENDF/B-VI Release	Material	ENDF/B-VI Release
Mo (Discarded)	0	W-182	0	U-235	4
Sm-149	0	W-183	0	U-236	0
Sm-150	2	W-184	0	U-238	2 (Modified)
Sm-152	2	W-186	0	Pu-238	0
Eu-151	0	Ir-191	4	Pu-239	2
Eu-152	0	Ir-193	4	Pu-240	2
Eu-153	0	Th-232	0	Pu-241	3
Eu-154	0	U-232	0	Pu-242	0
Ta-181 (Discarded)	0	U-233	0	Cm-244	0
Ta-182	0	U-234	0		

As noted in Table I, one evaluation was modified. The ^{238}U ENDF/B-VI Release 2 evaluation specifies an upper energy for the unresolved region of 300 keV. Unresolved data, however, are only provided up to 149.029 keV. To resolve this inconsistency, we changed the specified upper energy boundary of the unresolved region to 149.029 keV. (To be completely honest, this change was actually effected by changes made by hand to the processed NJOY file, not to the evaluation itself). In the subsequently available ENDF/B-VI Release 5 evaluation of ^{238}U, the upper energy of the unresolved region has indeed been changed to 149.029 keV, consistent with our modification here. This is not, however, the only change that has been made to the Release 5 evaluation.

NJOY processing

NJOY97 is a recent release of the NJOY nuclear data processing system. The code has undergone substantial modification in order to make it compatible with a much wider variety of compilers and computer hardware, both 32-bit and 64-bit systems. All processing for this work was performed with versions of NJOY97.

For each material, two major NJOY calculations are performed. Most of the work occurs during the first calculation, which we commonly refer to as the "PENDF run." This sequence utilizes the following modules of NJOY: RECONR, BROADR, UNRESR, HEATR, PURR, THERMR, and GASPR. This sequence begins by operating on the original ENDF/B-VI evaluation. RECONR reconstructs pointwise cross sections from resonance parameters and linearizes all cross sections on a unionized energy grid. BROADR generates Doppler-broadened cross sections using the kernel broadening method. UNRESR produces effective self-shielded cross sections for resonance reactions in the unresolved energy region. The HEATR module generates various quantities related to heat production and energy deposition. The PURR module is especially important for this work – it is in this module that the unresolved probability table data are generated. THERMR generates scattering cross sections in the thermal energy range. Finally, the GASPR module calculates production cross sections of hydrogen and helium isotopes.

The NJOY input file for the PENDF run for ^{235}U is reproduced in Appendix A. All materials were processed through NJOY using input files of this form and content. The parameters of particular importance to note are the 0.001 vales for fractional tolerances in both RECONR and BROADR. Also, note that the PURR input specifies 20 probability bins for each table, with each table to be generated based upon 32 unique resonance ladders. The final comment to make about the NJOY input file shown in Appendix A is that it creates as its output a file that is very general in nature -- much more general, in fact, than required specifically for this work. For example, the multiple temperatures and sigma zero values are not required in this work, and the UNRESR and THERMR modules could have been omitted entirely if the only objective was to generate a file for the MCNP URES library.

The second NJOY calculation is what we commonly refer to as the "ACER run." The major task accomplished during this sequence is to reformat the previously generated data into a form that is directly useful to MCNP. Error checking and consistency checks are performed during this sequence. Interpreted listings and plots are also generated. The NJOY input file for the ACER run for ^{235}U is reproduced in Appendix B. All cross sections on the MCNP library described in this Research Note are at 300 degrees Kelvin. As in the example in Appendix B, no thinning of the energy grid was performed during the ACER runs.

Table II provides a detailed list of exactly which version of NJOY97 was used in the PENDF run and ACER run for each of the 29 materials processed. The table also includes the date of the various calculations. All PENDF runs were performed on a Sun workstation whereas all ACER runs were performed on a Cray.

Table II

Versions and Dates of NJOY Processing

Material	NJOY Version for PENDF Run	Date of PENDF Run	NJOY Version for ACER Run	Date of ACER Run
Mo (Discarded)	97.15	8/18/98	97.9	8/18/98
Sm-149	97.13	8/14/98	97.9	8/15/98
Sm-150	97.13	8/14/98	97.9	8/15/98
Sm-152	97.13	8/14/98	97.9	8/15/98
Eu-151	97.13	8/14/98	97.9	8/15/98
Eu-152	97.13	8/14/98	97.9	8/15/98
Eu-153	97.13	8/15/98	97.9	8/15/98
Eu-154	97.13	8/15/98	97.9	8/15/98
Ta-181 (Discarded)	97.13	8/18/98	97.9	8/18/98
Ta-182	97.13	8/18/98	97.9	8/18/98
W-182	97.13	8/14/98	97.9	8/15/98
W-183	97.13	8/14/98	97.9	8/15/98
W-184	97.13	8/14/98	97.9	8/15/98
W-186	97.13	8/14/98	97.9	8/15/98
Ir-191	97.13	8/18/98	97.9	8/18/98
Ir-193	97.13	8/18/98	97.9	8/18/98
Th-232	97.15	8/16/98	97.9	8/16/98
U-232	97.17	8/27/98	97.9	8/27/98
U-233	97.3	5/28/98	97.9	8/16/98
U-234	97.13	8/15/98	97.9	8/15/98
U-235	97.13	8/16/98	97.14	8/28/98
U-236	97.13	8/15/98	97.9	8/16/98
U-238	97.13	8/16/98	97.14	8/28/98
Pu-238	97.10	7/4/98	97.6	7/6/98
Pu-239	97.13	8/15/98	97.9	8/17/98
Pu-240	97.11	8/13/98	97.9	8/16/98
Pu-241	97.11	8/14/98	97.9	8/16/98
Pu-242	97.11	8/14/98	97.9	8/16/98
Cm-244	97.15	8/17/98	97.9	8/17/98

Verification

URES contains nearly 5 million words of data. The prospect of verifying every piece of data, on a word-by-word basis, is not practical. Instead, we rely on a number of methods we have developed in the past to verify continuous-energy MCNP data tables and one new code written expressly for verifying the new PT data.

We will first list the traditional verification techniques employed in this work (see Ref. 11 for more details):

- NJOY performs several consistency checks during the second execution of the ACER module shown in Appendix B. The code checks several attributes of reaction thresholds, energy grids, and secondary energy and angular distributions. It flags anything known to be wrong or considered likely to be unreasonable. All 29 materials passed these internal consistency checks. In addition, we examined all NJOY output files for "messages" generated by the code during the execution of the various modules. All such messages were understood and were considered to be of minor consequence.

- Plots of each individual cross section for every isotope on URES were generated with the XSPLOT code (an updated version of XDATAP[12]). Each of the 764 plots was displayed and examined for signs of possible processing errors. None were identified, although energy-balance problems in the original evaluations led to negative heating numbers at certain neutron energies for ^{151}Eu, ^{183,184}W, ^{191,193}Ir, and ^{232}Th. The plots have been archived as a postscript file.

- The WHALE code[13] was used to calculate average cross sections in several energy ranges for each reaction from both the original ENDF/B-VI evaluation and from the final MCNP data table as processed by NJOY. Comparisons were made. All differences reported by WHALE (above a minimal tolerance level) were easily understood and deemed reasonable.

- Several small, special-purpose checking codes were executed. These codes are described in more detail in Ref. 11. No problems were identified.

The incorporation of probability tables is a major addition to MCNP data sets and a relatively untested feature of NJOY. As such, we wrote a new code specifically to perform a variety of consistency tests on the PT data. The code is named check_ures.

Check_ures does the following for each PT on an MCNP library:

- Ensures that any competition reaction specified (see the format description in Appendix C) actually exists.

- Checks the infinitely-dilute total cross section at the energy of the PT against the sum of the infinitely-dilute elastic, fission, capture, and competition cross sections. Fractional differences greater than 1.e-06 are noted.

- Checks to make sure that the cumulative probabilities as given in the PT are in ascending order, and that the distribution is correctly normalized to 1.

- Checks for negative values of the total, elastic, fission, and capture cross sections in each row of the PT. In addition, checks for zero cross sections for total, elastic, and capture.

- Checks for zero or negative values of the heating numbers in each row of the PT. Also warns if the value of a particular heating number is greater than some reasonable upper limit (chosen to be 210 MeV/collision).

- For each row, compares the total cross section from the PT with the sum of the elastic, fission, capture, and competition cross sections. Differences greater than 1% are noted.

- For each cross section (total, elastic, fission, capture, and heating), compares the infinitely dilute value at that neutron energy with the apparent average value from the PT. The infinitely dilute value is obtained from the traditional portion of the data table. The average value from the PT is obtained by summing the product of the differential probability and the cross section over each row. Fractional differences greater than 1.e-04 are noted.

One class of problem identified by check_ures led to the decision to exclude Mo and ^{181}Ta from the MCNP library. For both materials, a large number of negative cross sections were found in the PT data. Upon further review, the problems were traced to negative background cross sections in the ENDF/B-VI evaluations. These negative backgrounds are not an issue when only calculating infinitely dilute cross sections. They do, however, pose an unrealistic challenge to a processing code attempting to generate probability tables. Thus, we decided to drop plans to include data for Mo and ^{181}Ta on this library. This is the reason that, although we processed 29 materials, only 27 survived on URES.

Other problems identified by check_ures reflected upon the processing. Consequently, several iterations of NJOY processing resulted. In fact, the "final" NJOY processing as summarized in the previous section still led to some complaints from check_ures. They were:

- ^{152}Sm had small differences between the infinitely-dilute total and the sum of the infinitely-dilute partials. This issue resulted from the fact that NJOY97.9 neglected the competition cross sections from MT=22 and MT=107. These cross sections, while small, are non-zero over portions of the unresolved energy range. Instead of re-running NJOY, we directly modified the file produced to include MT=22 as an inelastic competition reaction and MT=107 as an absorption competition reaction. In addition, NJOY was updated so that it would include these competition reactions in the future.

- Two materials (^{232}Th and ^{241}Pu) each had one row in one PT with a zero differential probability. The same row also included non positive cross sections. Although this is not a desirable situation, it is not capable of damaging an MCNP calculation (since the row in doubt will never be sampled) and effectively means only that these two probability tables have 19 rows instead of 20. No changes were made.

- Several cases were identified for rows in which the total did not equal the sum of the partials. This check was made at the 1% level; it was repeated at a 5% level and no such disagreements were found. We believe that the apparent discrepancies result from the fact that NJOY normalizes each partial cross section and the total cross section (within a particular PT) independently from one another. As implemented in MCNP, the total cross section within the unresolved range is always calculated as the sum of the partials (i.e., the total cross section in the PT is never used directly). Therefore, we decided that no changes were necessary in this matter.

- Non-physical values of heating numbers were found in several cases for ^{232,233}U and ^{238,241}Pu. Values greater than 2900 MeV/collision were found. It should be emphasized that the average heating number from each PT was consistent with the infinitely-dilute value. However, one of us (RCL) believes that distributions of heating numbers that include such extremely large values are indicative that further work is required in this area. No changes were made at this time, however. *We warn users to be somewhat careful about MCNP F6 tallies calculated using this library.*

Finally, we are in the process of collaborating with KAPL and ANL to further verify the data in our probability tables. Both Laboratories have generated PT data from the same underlying evaluations, but by methods independent of NJOY. Thus, similarities between PT data from other Laboratories would lend additional confidence to our PT data; differences would require further investigation. This collaboration is only in its infancy; however, preliminary comparisons with KAPL PT data have been very encouraging. Results of this study will be reported at a later date.

MCNP Library

Data for the 27 isotopes were combined on to one library, named URES. Some characteristics of each data table are listed in Table III. All data have been processed at 300 degrees Kelvin. All ZAIDs on URES end in .49c.

Versions of the URES library (and associated directory files) for MCNP have been stored on CFS at Los Alamos. All files are under the /x6data/ce/special/probtable sub-directory. The relevant files are listed in Table IV. All of the files listed in Table IV were written to CFS on 10/05/98. All of the directory files listed in Table IV are "partial" directory files. That is, they contain entries for each of the 27 data tables, but nothing else. These directories need to be merged in to existing "full" directory files. Finally, all major files used in the creation of URES have been archived on CDROM.

The format of the PT data as contained in MCNP data tables has been previously documented by Lee Carter and John Hendricks (see Ref. 14). For completeness, we reproduce here in Appendix C the PT format description taken almost identically from Ref. 14.

Relationship to Other MCNP Libraries

Currently, the only generally-distributed MCNP library based upon ENDF/B-VI is ENDF60.[15] ENDF60 was distributed in 1994 and contains data for 122 nuclides based on ENDF/B-VI Release 2. All of the ZAIDs on ENDF60 end in .60c. Of the 27 isotopes on URES, seven were not available on ENDF60. Thus, URES represents our first ENDF/B-VI release for ^{149,150,152}Sm, ^{152,154}Eu, and ^{191,193}Ir.

Table III

Characteristics of Data Tables on the URES Library

Material	ZAID	Length of Data Table	Number of Energies	Photon Production Data	Minimum Probability Table Energy (keV)	Maximum Probability Table Energy (keV)
Sm-149	62149.49c	57,787	7,392	No	0.1	10.
Sm-150	62150.49c	60,992	8,183	No	1.6	100.
Sm-152	62152.49c	203,407	19,737	No	5.025	100.
Eu-151	63151.49c	147,572	10,471	Yes	.09881	1.
Eu-152	63152.49c	81,509	6,540	No	.0615	3.
Eu-153	63153.49c	129,446	8,784	Yes	.09722	1.
Eu-154	63154.49c	72,804	6,627	No	.063	10.
Ta-182	73182.49c	20,850	2,463	No	.035	10.
W-182	74182.49c	150,072	16,495	Yes	4.5	100.
W-183	74183.49c	119,637	12,616	Yes	0.765	45.
W-184	74184.49c	97,118	9,794	Yes	2.65	100.
W-186	74186.49c	102,199	10,485	Yes	3.2	100.
Ir-191	77191.49c	83,955	8,976	Yes	0.16	10.
Ir-193	77193.49c	82,966	8,943	Yes	0.3	10.
Th-232	90232.49c	305,942	41,414	Yes	4.	50.
U-232	92232.49c	21,813	2,820	No	0.053	1.
U-233	92233.49c	47,100	4,601	Yes	0.06	10.
U-234	92234.49c	161,296	22,539	No	1.5	100.
U-235	92235.49c	647,347	72,649	Yes	2.25	25.
U-236	92236.49c	159,074	20,865	No	1.5	100.
U-238	92238.49c	705,623	85,021	Yes	10.	149.03
Pu-238	94238.49c	41,814	5,337	No	0.2	10.
Pu-239	94239.49c	595,005	64,841	Yes	2.5	30.
Pu-240	94240.49c	341,542	41,596	Yes	5.7	40.
Pu-241	94241.49c	155,886	17,753	Yes	0.3	40.2
Pu-242	94242.49c	130,202	14,922	Yes	0.986	10.
Cm-244	96244.49c	97,975	11,389	Yes	0.525	10.

Table IV

Versions of URES and Directories Under /x6data/ce/special/probtable CFS Node

File Name	Description	Length (MB)
URES1	Type-1 version of URES	97.6
URES1.XS	Directory file for URES1	
URES2.UCOS	Type-2 version of URES for UNICOS	38.7
URES2.XS.UCOS	Directory file for URES2.UCOS	
URES2.UNIX	Type-2 version of URES for UNIX (32-bit)	19.4
URES2.XS.UNIX	Directory file for URES2.UNIX	

The other 20 isotopes on URES have MCNP cross-section tables on both ENDF60 (ZAIDs ending in .60c) and on URES (ZAIDs ending in .49c). In no case are the equivalent pairs of data tables identical (even accounting for the obvious addition of PT data on URES relative to ENDF60). One reason is that, for a couple of isotopes (namely ^{235}U and ^{241}Pu), the URES table is based on a later ENDF/B-VI release than the corresponding ENDF60 table. The more pervasive reasons for differences between URES and ENDF60 (even when the original evaluation source was identical) are that different versions of NJOY were used and that different parameters were used in the NJOY processing. For example, the 0.001 fractional tolerances used in the current NJOY processing are, in general, tighter than the tolerances previously used to generate the data on ENDF60. One manifestation of this difference in processing strategy is that the number of energy points used to represent the ^{239}Pu cross sections is 64,841 on URES, compared to 26,847 on ENDF60. Another major difference between URES and ENDF60 is that gas-production cross sections (MTs 203-207) and damage cross sections (MT=444) exist on URES; they do not on ENDF60. In summary, the MCNP data tables on URES are much more detailed in *many* respects than their counterparts on ENDF60, not just in the addition of PT data.

Los Alamos plans to release a major new MCNP neutron cross section library in 1999. The library is tentatively named ENDF65, which is to indicate that it will be based upon ENDF/B-VI Release 5 evaluations. ENDF65 will be a much more complete library than URES, providing cross sections for well over 100 materials. Data tables on ENDF65 for all materials whose evaluations provide unresolved resonance data will contain probability tables. Thus, the number of PT materials on ENDF65 will be larger than the limited set of 27 provided on URES.

Users should not anticipate that data for those materials common to URES and ENDF65 will be identical. One reason is that URES is based upon ENDF/B-VI Release 4 whereas ENDF65 will be based upon ENDF/B-VI Release 5. Some of the evaluations for materials on URES (for example, ^{235}U and ^{238}U) will be updated for Release 5. In addition, a later version of NJOY than used in this work will be used for the entire ENDF65 processing, and a slightly different processing strategy will likely be followed. Even for those materials without updated evaluations, we will assign new ZAID identifiers for each table on ENDF65. Because of this, we consider URES to be an interim library that will be superseded when ENDF65 is released.

Utilization in MCNP

Probability-table data will be used for neutron transport in MCNP only in Versions 4XS and later. Version 4XS is an intermediate version between MCNP4B and MCNP4C and is documented in Ref. 8.

With respect to PT data, the default in MCNP4XS is to use such data whenever they are available. The presence and use of PT data can be confirmed in print table 100 of the MCNP "outp" file by a statement associated with each relevant data table indicating "probability tables used from 2.25e-03 to 2.5e-02 MeV" (or whatever the minimum and maximum energies of the PT data are).

Users are allowed to turn off PT data in MCNP4XS by entering a non zero value for the third variable on the PHYS:N card. The code will then print a warning message indicating that "unresolved resonance probability tables turned off." When PT data are disabled by the user, MCNP reverts to its historical treatment of cross sections in the unresolved energy range. Users are encouraged to *not* routinely disable PT data; the predominant reason for doing so should be to determine the sensitivity of a particular calculated result to the unresolved data.

Data tables such as those found on URES may be used with versions of MCNP that predate the inclusion of a PT treatment (e.g., MCNP4B). However, the PT data will be ignored by the code in such cases, except that a slight increase in memory will be required.

As noted in Ref. 8, the format of xsdir entries for tables with PT data has been changed to include 'ptable' after the existing temperature entry. Users converting a type-1 representation of URES to a type-2 binary format *must* do so with a version of the MAKXSF auxiliary code that has been updated to recognize and include this new entry.[16] Otherwise, the resulting xsdir will not include the required 'ptable' entries.

Testing in MCNP

The majority of calculations reported to date using the PT method in MCNP have been performed with a version of MCNP preliminary to MCNP4XS and with a version of a cross-section library preliminary to URES. Nevertheless, these results may be of interest; we will therefore summarize them here.

Ref. 7 includes results of sample problems that were calculated with and without PT data. The problems were somewhat contrived, in that they were designed to emphasize unresolved region effects. Two shielding problems and one eigenvalue problem were described. The conclusion from the shielding problems was that neutron transmission through deep-penetration problems could be significantly increased in the unresolved region when PT data were used. The eigenvalue problem was designed to emphasize neutrons in the ^{238}U unresolved energy range; by doing this, a relatively significant increase in the eigenvalue was obtained as a result of the decrease in ^{238}U capture effected by using PT data. Although these calculations were based upon ENDF/B-V PT data and an interim version of MCNP, the general nature of the conclusions is not expected to change.

Refs. 17 and 18 include calculated results for several uranium and plutonium benchmark critical assemblies. Again, although these results were generated with preliminary versions of the code and data, we are confident that the conclusions based upon the results are valid. The major conclusion, in terms of impact of PT data, was that the method could produce substantial increases in reactivity for systems that include large amounts of ^{238}U and have high fluxes within the unresolved resonance region. Therefore, these results indicated that calculations for such systems would produce significantly non conservative results unless the PT method is employed. Unfortunately, agreement between calculations and experiments was actually worse when PT data were used. This disparity suggests that the unresolved resonance data for ^{238}U may need to be revised.

Finally, we have repeated calculations for three of the critical assemblies studied in Refs. 17 and 18 using URES and MCNP4XS. The assemblies are BIG TEN, ZEBRA-8B, and HISS/HPG (see Ref. 17 or 18 for details on these assemblies). Results from current calculations are compared with results reported in Ref. 18 in Table V (uncertainties shown are one standard deviation). Current calculations were performed on a Sun Ultra workstation. All current results are within two standard deviations of the results reported in Ref. 18.

Table V

Results for Selected Critical Assembly Benchmarks

Benchmark Name	Benchmark k_{eff}	Calculation Description	Calculated k_{eff} with PT data	Calculated k_{eff} without PT data	Δk_{eff} (PT – no PT)
BIG TEN	0.9960 (.0030)	Ref. 18	1.0112 (.0005)	1.0069 (.0005)	0.0043 (.0007)
		MCNP4XS and URES	1.0125 (.0005)	1.0077 (.0005)	0.0048 (.0007)
HISS/HPG	1.0000 (.0100)	Ref. 18	1.0115 (.0005)	1.0132 (.0006)	-0.0017 (.0008)
		MCNP4XS and URES	1.0119 (.0005)	1.0126 (.0006)	-0.0007 (.0008)
ZEBRA-8B	1.0010 (.0023)	Ref. 18	1.0177 (.0004)	1.0045 (.0005)	0.0132 (.0006)
		MCNP4XS and URES	1.0169 (.0004)	1.0056 (.0004)	0.0113 (.0006)

Availability

MCNP4XS and URES are *not* generally available to the worldwide MCNP user community. The reason is straightforward. The PT data on URES and functionality in MCNP4XS were developed largely under the support of the USDOE Nuclear Criticality Safety Program (NCSP), in particular through funding from DOE-EM. Another major MCNP4XS feature, enhanced criticality perturbation, was also developed under this support. Therefore, the distribution of MCNP4XS and URES has been put on a "fast track" primarily for the DOE nuclear criticality safety community.

Appropriate users from outside Los Alamos should contact the Radiation Shielding Information Computational Center (RSICC) at Oak Ridge to obtain MCNP4XS and URES. To contact RSICC, send e-mail to pdc@ornl.gov or telephone 423-574-6176.

All internal Los Alamos users may obtain access to both MCNP4XS and URES. For access to URES, send e-mail to nucldata@lanl.gov.

Other users will be able to access the capabilities embodied in MCNP4XS and URES when MCNP4C is made available for general distribution via RSICC. This distribution is currently anticipated in mid-late 1999.

Summary

This Research Note describes the first formal neutron library for MCNP that includes probability-table data to allow modeling of unresolved resonance self-shielding. The library, URES, was generated by the NJOY processing code based upon ENDF/B-VI Release 4. Data for 27 materials are included on URES, which is compatible with MCNP4XS and subsequent versions. The library has undergone significant verification. Only a modest amount of code / library validation has been presented here. The distribution policy for URES is that it is immediately available to the DOE nuclear criticality safety community (via RSICC) and to all users at Los Alamos.

Acknowledgments

We wish to acknowledge that this work was sponsored as part of the DOE Nuclear Criticality Safety Program (NCSP). In particular, the funding was made possible by the Office of Environmental Management (EM) at DOE and by the Program Manager, Dennis Cabrilla.

Lee Carter and John Hendricks are responsible for the code development that led to the probability-table method as included in MCNP4XS. In addition, Lee did much of the initial testing of cross-section tables from NJOY. Russ Mosteller has performed most of the more recent calculations.

We appreciate Bernadette Kirk and RSICC for agreeing to distribute MCNP4XS and URES to the nuclear criticality safety community.

Feedback from Stephanie Frankle and Pat Mendius on earlier drafts of this report have improved the final version.

Finally, the developing collaboration with KAPL and ANL on probability-table data can only make all of our capabilities stronger in the future. We wish to acknowledge the roles of Tom Sutton at KAPL and Roger Blomquist at ANL in this collaboration.

References

1. Judith F. Briesmeister, Editor, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 4B," LA-12625-M, Los Alamos National Laboratory (March 1997).

2. V. McLane, C. L. Dunford, and P. F. Rose, "ENDF-102, Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," BNL-NCS-44945, Revised, Brookhaven National Laboratory (November 1995).

3. Leo B. Levitt, "The Probability Table Method for Treating Unresolved Neutron Resonances in Monte Carlo Calculations," *Nucl. Sci. Eng.,* **49**, 450 (1972).

4. R. N. Blomquist, R. M. Lell, and E. M. Gelbard, "VIM – A Continuous Energy Monte Carlo Code at ANL," Proceedings of a Seminar-Workshop, A Review of the Theory and Application of Monte Carlo Methods, April 21-23, 1980, Oak Ridge, Tennessee, ORNL/RSIC-44.

5. T. M. Sutton and F. B. Brown, "Implementation of the Probability-Table Method in a Continuous-Energy Monte Carlo Code System," in Proceedings of International Conference on the Physics of Nuclear Science and Technology, Long Island, NY, Vol. 2, pp. 891-898 (1998).

6. S. H. Zheng, T. Vergnaud, and J. C. Nimal, "Neutron Cross-Section Probability Tables in TRIPOLI-3 Monte Carlo Transport Code," *Nucl. Sci. Eng.*, **128**, 321 (1998).

7. Lee L. Carter, Robert C. Little, John S. Hendricks, and Robert E. MacFarlane, "New Probability Table Treatment in MCNP for Unresolved Resonances," in Proceedings Of 1998 ANS Radiation Protection and Shielding Division Topical Conference, Nashville, TN, Vol. 2, pp. 341-347 (1998).

8. John S. Hendricks, "MCNP4XS," XCI-RN:JSH-98-044, Los Alamos National Laboratory Research Note (October 1998).

9. P. F. Rose, Compiler and Editor, "ENDF-201, ENDF/B-VI Summary Documentation," NNL-NCS-17541, Brookhaven National Laboratory (October 1991).

10. R. E. MacFarlane and D. W. Muir, "The NJOY Nuclear Data Processing System, Version 91," LA-12740-M, Los Alamos National Laboratory (October 1994).

11. S. Frankle, "Experience with ENDF60 and QA of a Continuous-Energy Library," XTM:SCF-96-363, Los Alamos National Laboratory Internal Memorandum (Sept. 23, 1996).

12. H. M. Fisher, "XDATAP," LA-11155-MS, Los Alamos National Laboratory (1988).

13. N. D. Keen, "WHALE, an Updated Version of MARK/MRKACR," XTM:95-253, Los Alamos National Laboratory Internal Memorandum (1995).

14. John S. Hendricks, "Proposed MCNP4C Manual Revisions," XCI:JSH-98-99 Rev. 1, Los Alamos National Laboratory Internal Memorandum (July 1, 1998).

15. John S. Hendricks, Stephanie C. Frankle, and John D. Court, "ENDF/B-VI Data for MCNP," LA-12891, Los Alamos National Laboratory (December 1994).

16. Andrew K. Hess, "Proposed Revision of MAKXSF for Correct Translation of Cross-Section Directories," XCI:AKH-98-97, Los Alamos National Laboratory Internal Memorandum (June 25, 1998).

17. Russell D. Mosteller and Robert C. Little, "Impact of MCNP Unresolved Resonance Probability-Table Treatment on Uranium and Plutonium Benchmarks," *Trans. Am. Nucl. Soc.*, **79**, 313 (1998).

18. Russell D. Mosteller and Robert C. Little, "Impact of MCNP Unresolved Resonance Probability-Table Treatment on Uranium and Plutonium Benchmarks," LA-UR-98-5192, Los Alamos National Laboratory, submitted to Sixth International Conference on Nuclear Criticality Safety (1998).

Distribution

Internal LANL Distribution:

X-DO File, MS B218

R. Krajcik / P. Soran / W. Krauser, X-DO, MS B218

X-CI File, MS F663

D. Shirk, X-CI, MS F663

A. Heath, X-CI, MS F663

R. MacFarlane, T-2, MS B243

M. Chadwick, T-2, MS B243

D. Madland, T-2, MS B243

P. Young, T-2, MS B243

S. Frankle, X-CI, MS F663

J. Campbell, X-CI, MS F663

J. Comly, X-CI, MS F663

C. Werner, X-CI, MS F663

M. White, X-CI, MS F663

K. Adams, X-CI, MS F663

F. Brown, X-CI, MS F663

T. Booth, X-CI, MS F663

J. Briesmeister, X-CI, MS F663

D. Court, X-CI, MS F663

L. Cox, X-CI, MS F663

J. Favorite, X-CI, MS F663

A. Forster, X-CI, MS F663

J. Hendricks, X-CI, MS F663

G. McKinney, X-CI, MS F663

R. Prael, X-CI, MS F663

G. Estes, X-TM, MS D409

R. Roberts, X-TM, MS D409

W. Urban, X-TM, MS D409

S. Becker, X-TA, MS B220

C. Lebeda, X-TA, MS B220

L. Rauber, X-NH, MS F664

D. Wade, X-NH, MS F664

R. Brewer, ESH-6, MS F691

C. Harmon, ESH-6, MS F691

D. Hayes, ESH-6, MS F691

T. McLaughlin, ESH-6, MS F691

S. Monahan, ESH-6, MS F691

S. Vessard, ESH-6, MS F691

P. Jaegers, NIS-6, MS J562

R. Mosteller, NIS-6, MS J562

R. T. Perry, NIS-7, MS E541

E. Pitcher, LANSCE-12, MS H816

G. Russell, LANSCE-12, MS H805

External Distribution:

D. Cabrilla, DOE-EM

L. Carter, Carter MC Associates

B. Kirk, ORNL

R. Roussin, ORNL

M. Westfall, ORNL

R. Blomquist, ANL

E. Fujita, ANL

T. Sutton, KAPL

Appendix A - NJOY INPUT File for “PENDF Run” for ^{235}U

```
moder
 20 -21
 reconr
 -21 -22
 'pendf tape for endf/b-vi.4 u-235'/
 9228 9/
 .001/
 '92-u-235 from endf/b-vi.4'/
 'processed with njoy 97.9'/
 'the following reaction types are added'/
 '     mt152   bondarenko unresolved'/
 '     mt153   unresolved probability tables'/
 '     mt20x   gas production'/
 '     mt221   free thermal scattering'/
 '     mt301   total heating kerma factor'/
 '     mt443   kinematic kerma'/
 0/
 broadr
 -21 -22 -23
 9228 9 0 1/
 .001/
 300 400 600 800 1000 1200 1600 2000 3000/
 0/
 unresr
 -21 -23 -24
 9228 9 7 1
 300 400 600 800 1000 1200 1600 2000 3000/
```

```
1e10 1e4 1e3 300 100 30 10/
0/
heatr
-21 -24 -25/
9228 4/
302 318 402 443/
heatr
-21 -24 -22/
9228 6 0 1 0 2/
302 303 304 318 402 443
purr
-21 -25 -26
9228 9 7 20 32/
300 400 600 800 1000 1200 1600 2000 3000/
1e10 1e4 1e3 300 100 30 10/
0/
thermr
0 -26 -27
0 9228 8 9 1 0 1 221 0/
300 400 600 800 1000 1200 1600 2000 3000/
.005 4.5/
gaspr
-21 -27 -28
moder
-28 29
stop
```

APPENDIX B - NJOY INPUT File for “ACER Run” for ^{235}U

```
acer
 20 21 0 31 32
 1 0 1/
 '92-u-235 from endf-vi.4 njoy97.9'/
 9228 300./
 .01/
 /
 acer
 0 31 33 34 35
 7 1 2/
 '92-u-235 from endf-vi.4 njoy97.9'/
 viewr
 33 36/
 stop
```

APPENDIX C – Format Description for MCNP Probability-Table Data

This format description is intended to be included in Appendix F of the MCNP manual (Ref. 1).

If probability-table data exist; JXS(23) LUNR = location of probability tables

UNR Block --- contains the unresolved resonance range probability tables. The UNR block exists if JXS(23) > 0.

Format of UNR Block:

Location in XSS	Parameter	Description
JXS(23)	N	number of incident energies where there is a probability table.
JXS(23)+1	M	length of table; i.e., number of probabilities, typically 20.
JXS(23)+2	INT	interpolation parameter between tables; =2 lin-lin; =5 log-log
JXS(23)+3	ILF	inelastic competition flag (see below)
JXS(23)+4	IOA	other absorption flag (see below)
JXS(23)+5	IFF	factors flag (see below)
JXS(23)+6	E(I),I=1,N	incident energies
JXS(23)+6+N	P(I,J,K)	probability tables (see below)

ILF is the inelastic competition flag. If this flag is less than zero, the inelastic cross section is zero within the entire unresolved energy range. If ILF is greater than zero, then it is a special MT number whose tabulation is the sum of the inelastic competition reactions. An exception to this scheme is typically made when there is only one inelastic reaction within the unresolved energy range, since the flag can then just be set to the MT number of the reaction and a special tabulation is not needed. The flag can also be set to zero, which means that the sum of the contribution of the inelastic competition reactions will be made “on-the-fly” by MCNP using a balance relationship involving the smooth cross sections.

IOA is the other absorption flag for determining the contribution of "other absorptions" (no neutron out or destruction reactions). The "other" in "other absorptions" refers to absorption reactions other than radiative capture. If this flag is less than zero, the "other absorption" cross section is zero within the entire unresolved energy range. If IOA is greater than zero, then its value is a special MT number whose tabulation is the sum of the "other absorption" reactions. An exception to this scheme is typically made when there is only one "other absorption" reaction within the unresolved energy range, since the flag can then just be set to the MT number of the reaction and a special tabulation is not needed. The flag can also be set to zero, which means that the sum of the contribution of the "other absorption" reactions will be made "on-the-fly" by MCNP using a balance relationship involving the smooth cross sections.

IFF is the factors flag. If this flag is zero, then the tabulations in the probability tables are cross sections. If the flag is one, the tabulations in the probability tables are factors that must be multiplied by the corresponding "smooth" cross sections to obtain the actual cross sections.

P(I,J,K), where I=1,N, J=1,6, and K=1,M, are the tables at N incident energies for M cumulative probabilities. For each of these probabilities the J values are:

1 cumulative probability

2 total cross section or total factor

3 elastic cross section or elastic factor

4 fission cross section or fission factor

5 (n,γ) cross section or (n,γ) factor

6 heating number or heating factor

The ordering of the probability-table entries is as follows:

- M cumulative probabilities for energy I=1 (K=1 through K=M)
- M total cross sections (or factors) for energy I=1 (K=1 through K=M)
- …
- M cumulative probabilities for energy I=2 (K=1 through K=M)
- …
- M heating numbers (or factors) for energy I=N (K=1 through K=M)

Notes: The cumulative probabilities are monotonically increasing from an implied lower value of zero to the upper value of P(I,1,K=M) = 1.0. The total cross section, P(I,2,J), is not used in MCNP; the total is recalculated from sampled partials to avoid round-off error. The (n,γ) cross section is radiative capture only; it is not the usual MCNP "capture" cross section which is really absorption or destruction with other no-neutron-out reactions included.